The Correspondence Principle and Wavepackets

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One approach used in quantum mechanics to link it to classical physics for high energy eigenvalues, is the use of wavepackets. In this note, we examine a wavepacket approach, already existing in the literature, applied to the Bohr atom. We try to see if results obtained can be discerned without forming a wavepacket. In addition, we try to discuss the role played by classical physics in the quantum wavefunction and suggest that there is a cycling of""plane wave" momentum states with zitterbewegung in addition to classical physics for every energy eigenvalue, large or small. We argue that it is only when the energy eigenvalues become large that one sees sharp peaks in the spatial wavefunction, suggesting localization. (This localization is already well-known in the literature.) The localization allows one to see the classical information more clearly, but it is always present, as are the "quantum mechanical" features that lead to the peaks in the first place.Finally, we question the interference that occurs between wavefunctions used in the linear combination of a wavepacket.

Wavepacket Approach

The approach used to construct wavepackets seems to be the following. One first solves the time-independent Schrodinger equation to obtain eigenenergies and corresponding wavefunctions. One then chooses a set of high energy solutions (which tend to be closely spaced) and forms a linear combination of these with an "imposed" weight function. This leads to a localized wavefunction which is to represent a particle existing at a point in space. One then adds the factor exp(iEt) to each wavefunction in the packet to determine time dependence.

A question asked in this note is whether it is necessary to form a wavepacket to to obtain this information? A second question is: When did the classical type behaviour "turn on"?

It is known that adding the factor exp(iEt) to wavefunctions used in a linear combination tend to lead to an unwanted spreading of the overall wavefunction which is supposed to be localized at a point. As a result, some people use a completely different approach and seek soliton solutions which are already localized.

Wavepacket Approach to the Bohr Atom

In (1), a clear derivation of the wavepacket approach is applied to the Borh atom. The arguments seem to be as follows. First, a general wavefunction solution to the time-independent Schrodinger equation is given:

$$W_i(x) = R_{n,l}(r)\, Y_{lm}(\theta, \phi)$$

Here YLm(theta, phi) is the traditional spherical harmonic and n is an integer representing the energy level. Next, properties of the wavefunction are considered for the case of L=m, and n=L+1 which leads to simplifications.

1. First, the spherical harmonic is considered and it is noted that it behaves as $|\sin(\text{theta})|^2$ which is peaked at theta=pi/2. No restriction is placed on phi, so one can assume that it can move in a circle.
2. Next, Rn,L(r) which is a Laguerre solution, is examined for large n. This is where the ideal of large n appears and it is used because there are sharp peaks in the spatial wavefunction, and hence density, in such a case. It is found that the Laguerre result is peaked at an r* value proportional to .L(L+1) for n= L+1.
3. In (1), the next step is to construct a linear combination of such wavefunctions using a weight factor of one's choice. The result is a function peaked at r*, theta=pi/2 and phi=0.
4. The last step is to add the factor exp(iE(n)t) to each wavefunction in the linear combination and analyse the result to find group velocity.

The conclusion is that the particle tends to move in a circle with radius r* with a certain angular frequency.

In this note, we suggest this information can already be obtained at step 2. At this point, it is already known a high n wavefunction is peaked at r* and that theta=pi/2. Phi is left free, so the particle moves in a circle of r* at theta=pi/2. To calculate angular frequency, one can use classical conservation of energy, which we argue, exists for every eigensolution in quantum mechanics. Thus, "classical" results are not "turned on" for large energy eigenvalues.

Kinetic energy + potential energy = E

$E(L) = -E(g)/ [L+1]^2$

according to (1) with E(g) being the ground state energy. Now w=v/r where w is the angular frequency, thus:

$.5m\ w^2 r^{*2} + kq/r^* = -E(g)/ [L+1]^2$

And r* is proportional to (L+1)*(L+1) because one is using n=(L+1). Thus,

w* is proportional to $1/ [L+1]^3$

Or w* is proportional to $1/ [r^*]^{3/2}$

which is Kepler's law as pointed out in (1). The results are, however, obtained with no use of wavepackets.

Classical Physics in the Time Independent Schrodinger Equation

In (2), it is argued that the time-independent Schrodinger equation can be written as:

[Sum over p fp p*p/2m sin(px)] / W(x) + V(x) = E

Here W(x) is the wavefunction. Thus, classical conservation of energy exists for every eigenenergy in quantum mechanics. It does not seem to be the case that “classical” behaviour is “turned on” for large E. It seems, however, that two other important situations are occuring. First, there is a cycling over different p momentum values related to exp(iEt). A zitterbewegung type of particle, modeled by sin(px) which indicates that it can exist within a region of 1/p the wavelength) is scattered into various states by V(x). This scattering, however, forms a resonance with weight fp and a cycling through the states in a time 1/E as described by exp(iEt). For low energy E, it is difficult to discern any classical type motion, because the zitterbewegung sin(px) terms, with their interference features, tends to dominate. For high n, it is possible to have sharp peaks in the spatial wavefunction. The Bohr atom described above shows such a peak in a Laguerre solution, and Hermite polynomial solutions of the harmonic oscillator also show peaks for high n.

Let us see if these peaks can be linked to classical physics.In (1) it is noted that <W(x)|V(x)|W(x)> will take on the value V(x at peak) and so classical physics occurs. This seems to be the same as saying the particle is localized at these peaks, which makes it look classical. There can be numerous peaks in a high energy solution, such as in the oscillator case.

We note that for classical physics:

density(x) * v(x) = Constant (3)

For quantum mechanics:

-1/2m W(x) del*del W(x) = d(x) .5m v(x)*v(x)

Here W(x) is the wavefunction, v(x) the classical velocity and d(x)=W(x)*W(x), the density. Dividing by v(x) and setting the result equal to a constant yields:

-.5/m W(x) del*del W(x) = v(x) Constant

Now, -.5W(x)W(x) = (E-V(x)) W(x)W(x), so if W(x) is peaked at a point so is the kinetic energy density making the whole quantum problem look classical, even though momentum cycling and zitterbewegung are still occurring.

Interference in the Wavepacket Approach

The wavepacket approach using a linear combination of wavefunctions. This means that interference occurs between different wavefunctions (i.e additions and cancellations). In (2), it was argued that interference occurs during momentum cycling because, due to zitterbewegung, a particle moves back and forth while moving with average v in one direction. While undergoing the forward motion, it undergoes a positive reaction with V(x), but while moving backwards, a negative one. Thus, there may be a physical reason for interference. It is not clear that there is any physical reason to allow for interference in a wavepacket.

Conclusion

In conclusion, we argue that one can obtain the results of wavepackets without forming them. It seems that the results follow from high energy properties of the wavefunction. The high energy solutions tend to lead to spatial peaks. This make it look like the particle is localized and so classical. We argue, however, that classical physics is already present in the ground state, but difficult to see due to momentum state cycling and zitterbewegung These features are still present in high energy solutions, but peaks at certain positions make the problem look classical there. Finally, we question the physical grounds for allowing for interference between wavefunctions used in the linear combination needed to form a wavepacket.

References

1.Dhar, Deepak. The Bohr Correspondence Principle 2016
https://www.ias.ac.in/article/fulltext/reso/021/06/0565-0573
2. Ruggeri, Francesco R. Logarithm of Wavefunction as Partition Function (preprint, zenodo, 2018)
3.Majernik, V. and Opartny, T. Entropic Uncertainty Relations for a Harmonic Oscillator (J. Phys. A. Math 1996, 2187-2197).upol.cz/tom/clanky/jpa96-ent.pdf